

Benzeneethanimidamide, N-phenyl-  
7118-59-4 | DTXSID70221381

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 159 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.31e-01

Confidence level: 7.67e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>4,4'-Methylenedianiline</div> <div>Measured: 97.7</div> <div>Predicted: 87.8</div>	<div>Image not found</div> <div>4,4'-Thiodianiline</div> <div>Measured: 110</div> <div>Predicted: 116</div>	<div>Image not found</div> <div>MCPB</div> <div>Measured: 537</div> <div>Predicted: 245</div>
<div>Image not found</div> <div>N-(1,1-dimethyl-2-propynyl)-4-methoxybenzamide</div> <div>Measured: 67.6</div> <div>Predicted: 72.5</div>	<div>Image not found</div> <div>Ethyl 1-naphthaleneacetate</div> <div>Measured: 302</div> <div>Predicted: 425</div>	